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14. ABSTRACT
Our primary focus in this to apply the concept of cohesive zone models to link atomistic effect within a continuum based multi-scale model.
We have used this approach to consider the effect of interfaces in carbon nanotubes on the properties of CNT based polymer matrix composites.

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Annual Performance Report

FA9550-04-1-0202

Cohesive Zone Model Approach to Multiscale Modeling of Nanotube Reinforced Composites

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Research Objectives

Our primary objective in this research is to identify the mechanisms that can influence the load transfer mechanisms in carbon nanotube based composites using molecular dynamics simulations and develop a cohesive zone model to incorporate these atomic scale effects into a continuum finite element based model.

Approach

Carbon nanotubes (CNT), due to their excellent mechanical properties are proposed as next generation fibers for composite materials. In spite of the excellent mechanical properties of CNTs, the properties of CNT based composites are not as high as expected. Low interfacial strength could be a possible reason for this. We use combination of molecular dynamics and cohesive zone modeling to develop a hierarchical model which is employed for studying the interface effects.

Pullout test is typically used to characterize the interfacial behavior. It is extremely difficult to conduct single fiber pullout tests on CNTs because of their nanometer size. We have used molecular dynamics simulations of pullout tests using Tersoff-Brenner potential to characterize the interfacial behavior.

Specific approaches to the problem have been identified and preliminary results are presented in the attached slides. They include:

- Atomic simulations of nanotube pullout tests.
- Characterizing the interface behavior variation with different factors such as chemistry and temperature.
- Characterizing the interface behavior when CNTs interact with matrix only through Vanderwall's interactions
- Defining stresses and strains in nanotubes and studying the effect of hybridization and topological defects on CNTs.
- Identify the possible micromechanisms which affect the composites such as CNT curvature and perform simulations to incorporate these effects
- Developing a cohesive zone model that incorporates the atomic scale effects obtained from MD simulations

- Study of composite properties incorporate the effect of interfaces in the form of cohesive zone model.
- Develop analytical model to incorporate CZM into shear lag model.

Cohesive zone models (CZMs) can accurately characterize the mechanics of the fracture and failure process at the smallest scale. This research has established a link between micomechanics of the failure process with various deformation mechanisms to the macroscopically observed fracture. The method has been effectively to ductile, brittle materials and interfaces thereof.

Significance -Air force value

We expect our theory and computations to provide an understanding of the influence of the development and understanding of high strength light weight composite materials reinforced with nanoscale materials. We intend to develop a computational code, based on sound physics that is capable of describing the mechanical behavior of composites at various length scales using both molecular dynamics and finite element method. We

expect our ideas to be applicable to a plethora of elastic and inelastic deformation processes where micromechanics have a role to play. In addition, the multiscale model provides a method to incorporate atomic scale effects into continuum formulations and may be used for other generic applications of interest to army.

Accomplishments

As a part of the research effort we have

- Studied the tensile behavior of functionalized CNTs and determined that mechanical properties are not significantly affected by functionalization
- Performed atomic simulations of CNT pullout test with interface represented as hydrocarbon attachments. It is shown that such interfaces possess much higher strength than interfaces based on vanderwalls interactions.
- Above results are compared with CNT pullout with CNTs interacting only through vanderwalls interaction
- Developed cohesive zone model from atomic simulations
- FEM simulations using this atomically informed CZM
- Developed analytical model to incorporate imperfect interfaces into shear lag model.

Publications

During the past year articles related to this work published in journals, conference volume are listed below:

1. S Namilae and N Chandra, Multiscale model to study the effect of interfaces in nanotube reinforced composites, ASME Journal of Engineering Materials and Technology (Accepted) 2004

2. C. Shet, N. Chandra and S. Namilae, Defect-defect interaction in carbon nanotubes under mechanical loadings, Mechanics of Advanced Materials and Structures, (accepted) (2004).

3. C. Shet, N. Chandra and S. Namilae Defect annihilations in carbon nanotubes under thermo-mechanical loadings, Journal of Material Science, (accepted), (2004).

4. J. Kohle, U. Chandra, S. Namilae, A. Srinivasan and N. Chandra, Parallel simulation of Carbon Nanotube based composites. Proceedings of the 11 th International Conference on High Performance Computing (HiPC), Lecture Notes in Computer Science, Springer, 2004 (to appear).

5. N. Chandra and S. Namilae, Mechanics of Atomic Scale Interfaces in Carbon Nanotube Reinforced Composites,. Proceedings (CD) of the 2004 International Conference on Computational and Experimental Engineering and Sciences, Madeira, Portugal, 26-29 July '04, Advances in Computational and Experimental Engineering and Science, Ed., S. N. Atluri and AJB Tadeu, ISBN 0-9657001-6-X , pp 351-356, (2004)

6. N. Chandra and C, Shet, Modeling of CNT based composites, Numerical Issues, Proceedings (CD) of the 2004 International Conference on Computational and Experimental Engineering and Sciences, Madeira, Portugal, 26-29 July '04, Advances in Computational and Experimental Engineering and Science, Ed., S. N. Atluri and AJB Tadeu, ISBN 0-9657001-6-X, pp 1421-1426, (2004)

7. M Naveen, S Namilae, C. Shet and N. Chandra , Phase Space Distribution of Carbon Nanotubes in a Constant Temperature Molecular Dynamics Simulations, Proceedings of SECTAM XXII, Developments in Theoretical and Applied Mechanics, edited by Hassan Mahfuz and Mahesh V. Hosur, ISBN 0-615-12639-1, pp 1-11, (2004).

8. J. Kohle, U. Chandra, S. Namilae, A. Srinivasan and N. Chandra, Parallelization of Molecular Dynamics for Modeling Interface Properties of Carbon Nanotube Based Composites, Proceedings of SECTAM XXII, Developments in Theoretical and Applied Mechanics, edited by Hassan Mahfuz and Mahesh V Hosur, ISBN 0-615-12639-1, pp 23-32, (2004).

9. S. Namilae and N. Chandra, Three Level Hierarchical Model to Incorporate Interface Effects in Carbon Nanotube Based Composites, Proceedings of SECTAM XXII, Developments in Theoretical and Applied Mechanics, edited by Hassan Mahfuz and Mahesh V Hosur, ISBN 0-615-12639-1, pp 33-41, (2004).

10. N. Chandra, S. Namilae and A. Srinivasan, Linking Atomistic and Continuum Mechanics Using Multi-scale Models, Proceedings of the 8th International Conference on Numerical Methods in Industrial Forming Processes , Numiform 2004, AIP Conference Proceedings, Vol. 712, Issue 1, pp 1571-1576, June 13-17, Columbus, OH (2004)

11. A. Srinivasan and N. Chandra, Latency tolerance through parallelization of time in scientific application, Heterogeneous Computing Workshop, proceedings of the 18th International Parallel and Distributed Processing Symposium (IPDPS) April 2004, IEEE.

12. N. Chandra, S. Namilae, and C. Shet, Local elastic properties of carbon nanotubes in the presence of Stone -Wales defects, Physical Review B, 69, 094101, (2004)

13. S. Namilae, N. Chandra, and C. Shet, Mechanical behavior of functionalized nanotubes, Chemical Physics Letters, 387,247, (2004)

Mechanical behavior of functionalized nanotubes

How do fiber properties differ with chemical modification of surface?

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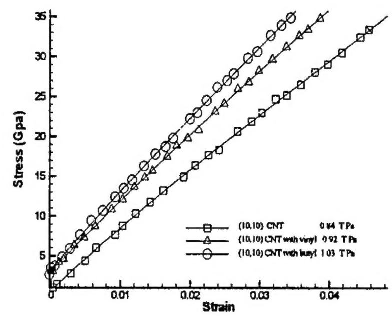
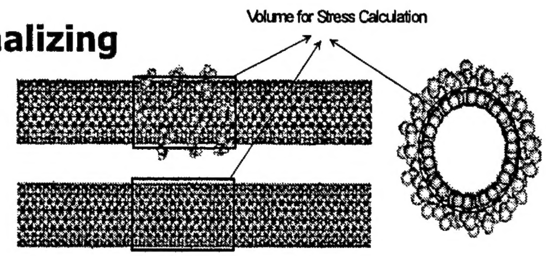
- Change in hybridization (SP2 to SP3)
- Experimental reports of different chemical attachments
- Application in composites, medicine, sensors

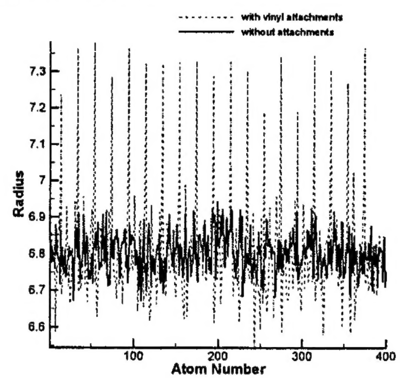
Methodology: (1)MD simulations based of Tersoff –Brenner potential. (2) Atomic level stress and strain measures

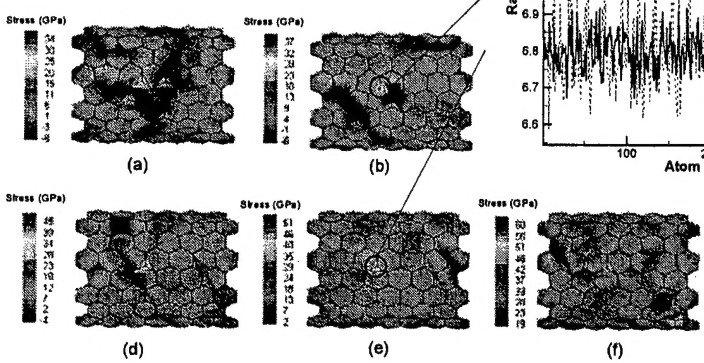
Increase in stiffness observed by functionalizing

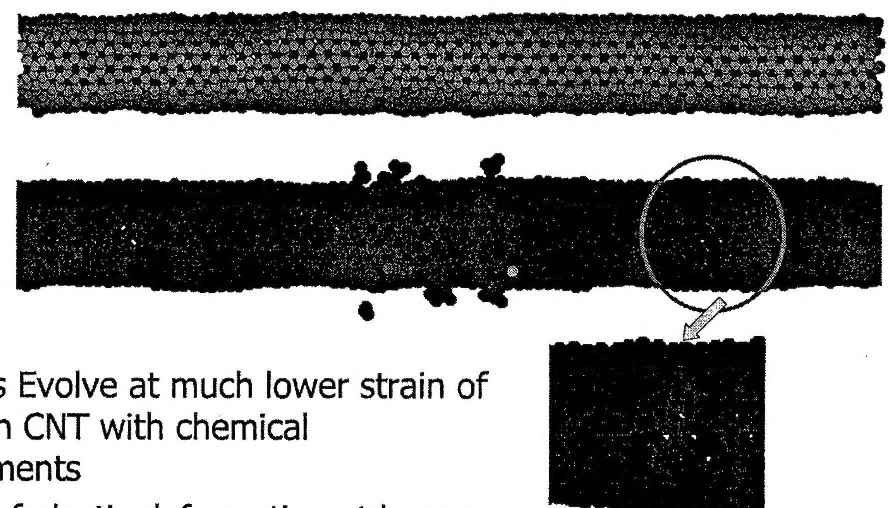


Stiffness increase is more for higher number of chemical attachments
Stiffness increase higher for longer chemical attachments









- Defects Evolve at much lower strain of 6.5% in CNT with chemical attachments
- Onset of plastic deformation at lower strain. Reduced fracture strain

POSSIBLE REASONS

- Serrations because of functionalization
- Sharp stress variations

Chemical Physics Letters (2004)

CZM based multiscale model for CNT composites

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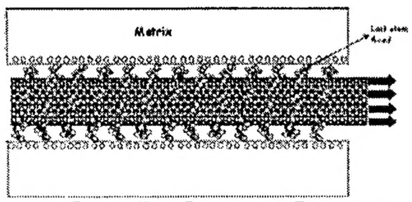
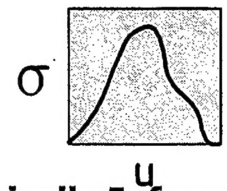
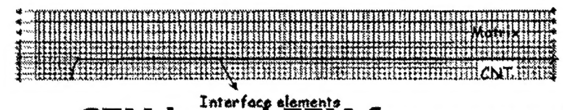


MD simulations of CNT Pullout



Atomically Informed CZM For interfaces

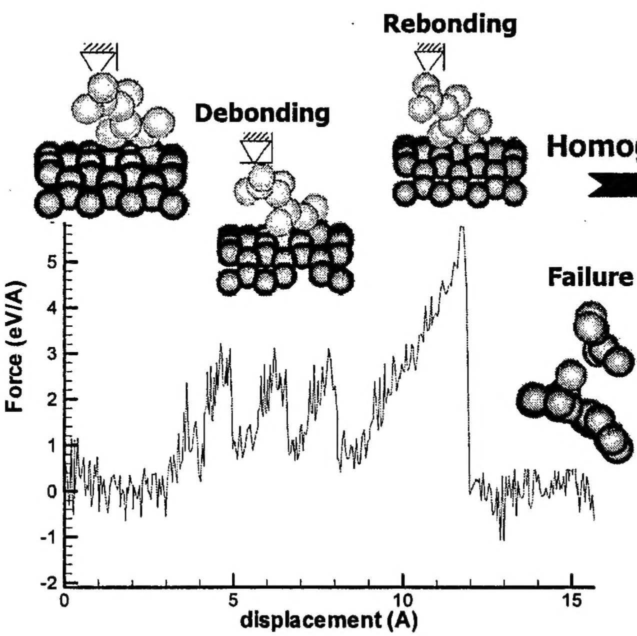


CZM based FEM for composite

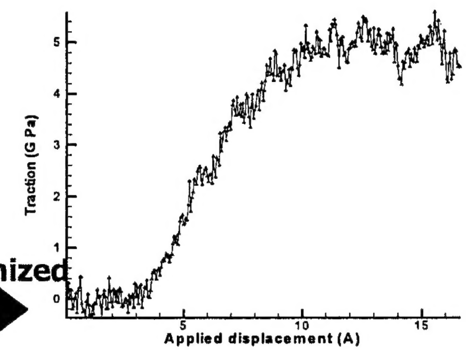
Simulation conditions:

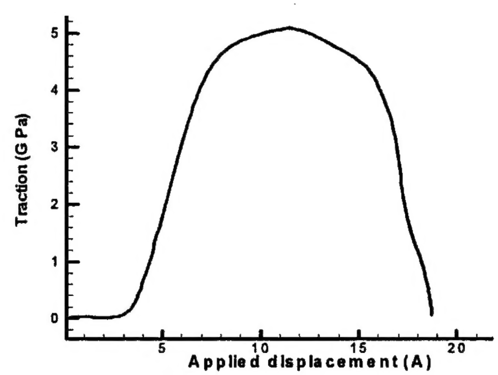
Corner atoms fixed, T=300K

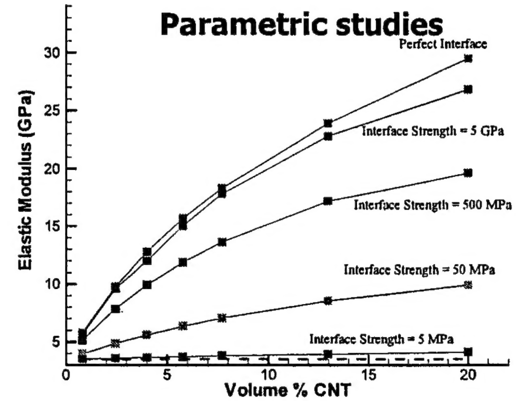
Displacement 0.02A/1500 steps

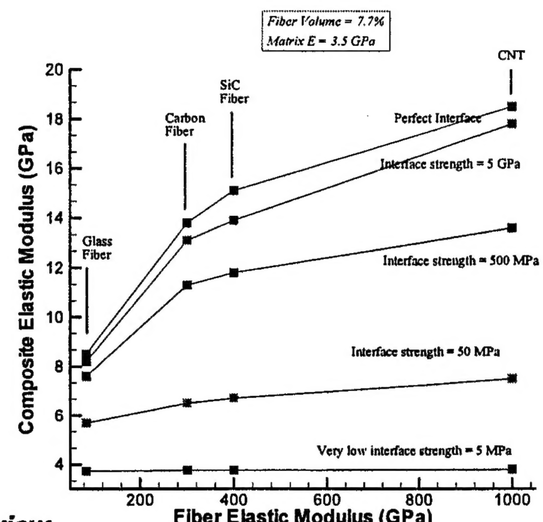


Homogenized









Interface strength as high as 5GPa possible by chemical linking

JEMT (2004) In Review